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ON THE SOLUTION OF A CONSTRAINED MINIMIZATION PROBLEM IN H'( $\Omega$ ) RELATED TO DENSITY ESTIMATION

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ON THE SOLUTION OF A CONSTRAINED MINIMIZATION PROBLEM IN H $^{1}(\Omega)$  RELATED TO DENSITY ESTIMATION

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#### ABSTRACT

In this paper we study the problem of the minimization of the Dirichlet integral over a two-dimensional domain, by non-negative functions satisfying a finite number of linear constraints. Existence and uniqueness of the solution is proved. A characterization by variational inequality is given, leading to local and boundary behaviour of the solution. This characterization is of importance in the construction of numerical algorithms for the production of non-negative smooth surfaces from aggregated data.

AMS (MOS) Subject Classifications: 41A63, 65D10, 35J25, 35J30

Key Words: Surface fitting, aggregated data, volume matching, optimization, elliptic variational inequalities, iterated Laplacian.

Work Unit Number 3 - Numerical Analysis and Computer Science

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#### SIGNIFICANCE AND EXPLANATION

The problem of constructing a smooth positive surface over a given domain, matching a set of data in aggregated form, as volumes over subdomains, is important in the estimation of densities. For example, given the population census according to political subdivisions (e.g. counties), it is desired to obtain a smooth positive function estimating the population density as a function of the geographical coordinates.

In order to select, from the infinitely many positive surfaces matching the data, a particular one which is smooth, we require the surface to minimize a Dirichlet-type integral, measuring the roughness of the surface over the domain. In this work we analyze the properties of the minimizing surface and characterize it by variational inequalities and also by its local differential behaviour in the domain and on its boundary.

This characterization is important in the construction of numerical methods for the production of discrete approximations to the minimizing surface and in the analysis of their convergence.

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## ON THE SOLUTION OF A CONSTRAINED MINIMIZATION PROBLEM IN H'( $\Omega$ ) RELATED TO DENSITY ESTIMATION

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Nira Dyn and Wing Hung Wong

## 1. Introduction

In this paper we are interested in the existence, uniqueness and characterization of the solution to the following minimization problem:

(1a) 
$$\min \mathbf{ze} \ J(\mathbf{u}) = \int_{\Omega} (\mathbf{u}_{\mathbf{x}}^2 + \mathbf{u}_{\mathbf{y}}^2) d\mathbf{x} d\mathbf{y}$$
 
$$\mathbf{u} \in H^+(\Omega)$$

subject to

(1b) 
$$\int_{\Omega} uf_{i} = \alpha_{i} , i = 1,...s ,$$

(1c)<sup>1</sup>) 
$$u > 0$$
 a.e. in  $\Omega$ ,

where  $\Omega$  is a smooth region in  $R^2$ ,  $f_i \in L^2(\Omega)$ , i = 1, ..., s, and  $H^*(\Omega)$  is the first order Sobolev space:

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In case  $\Omega$  has a smooth boundary, the non-negativity almost everywhere in (1c) is equivalent to non-negativity in the sense of  $H^1(\Omega)$  ( $u \ge 0$  in  $\Omega$  in the sense of  $H^1(\Omega)$ , if  $\Im\{\phi_n\} \subset C^1(\Omega)$   $\phi_n \ge 0$  in  $\Omega$ , such that  $\phi_n \to \phi$  in  $H^1(\Omega)$ ) (See e.g. Kinderlehrer and Stampacchia [6]).

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 $H^*(\Omega) = \{u \in L^2(\Omega): u_x, u_y \in L^2(\Omega)\}$  where  $u_x, u_y$  are the first order distributional derivatives.

This problem is of interest in the production of smooth contour maps from aggregated data (Dyn and Wahba [3]), and in particular for the estimation of a density from its given volumes

(1b)' 
$$\int_{\Omega_{\mathbf{i}}} \mathbf{u} = \alpha_{\mathbf{i}} , i=1,...,s$$

over a certain partition  $\Omega_1, \dots, \Omega_n$  of the domain  $\Omega_n$  (Tobler [7], Wahba [8].)

The familiar stationary obstacle problem in mechanics (Glowinski [5]) is similar to (1) without the linear constraints (1b).

In the following, we limit the discussion to sets of constraints (1b) satisfied by at least one smooth positive function. This is always the case for constraints of the form (1b) with  $\alpha_i > 0$ , i = 1, ..., s.

In section 2, we give a simple existence and uniqueness proof. Using results from optimization theory in Banach spaces, we have given in Section 3 a characterization of the solution in terms of a variational inequality. In Section 4, we combine the results of Section 2 and Section 3 with a theorem of P. H. Brezis [2] to study local properties of the solution. In particular the solution is found to be continuous and therefore non-negative everywhere in  $\Omega$ , two properties which are essential for applications.

These characterizations of the solution to (1) are of crucial importance in the construction of numerical procedures for the computation of the solution, and in establishing their convergence rates (Wong [9]). The analogous characterizations of the solution to the obstacle problem (1a) + (1c) are the basis to several numerical procedures for the computation of this solution (see Glowinski [5] for a review of these methods).

We conclude by considering in Section 5 similar minimization problems to (1), but with the functional in (1a) replaced by

$$J_{m}(u) = \int_{\Omega} \sum_{i=0}^{m} {m \choose i} \left( \frac{3^{m}u}{3x^{i} 3y^{m-1}} \right)^{2}.$$

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The results obtained are analogous to those for the case n = 1, with the exception of the local and boundary behaviour deduced from Brezis' result for n = 1.

This problem with m > 2 is of interest in the production of highly smooth surfaces fitting given aggregated data.

## 2. Existence and uniqueness

Theorem 1: There exists a unique solution to problem (1) whenever  $\sum_{i=1}^6 \left(\int_\Omega f_i\right)^2 > 0.$ 

<u>Proof:</u> Without loss of generality assume  $\int_{\Omega} f_1 = G \neq 0$ , and let  $u = u - \frac{1}{G} \alpha_1$ . Then (1) is equivalent to

(2a) 
$$\min \ \sigma(\widetilde{u}) = \int_{\Omega} \widetilde{u_X}^2 + \widetilde{u_Y}^2$$

subject to  $\widetilde{u} \in \widetilde{H'}(\Omega) = \{u \in H'(\Omega) \mid \int_{\Omega} uf_{\frac{1}{4}} = 0\}$  and

(2b) 
$$\int_{\Omega} f_{i} \tilde{u} = \alpha_{i} - \frac{G_{i}}{G} \alpha_{i} \text{ where } G_{i} = \int_{\Omega} f_{i}, i = 2, ..., s$$

(2c) 
$$\tilde{u} > -\frac{\alpha_1}{G}$$
 a.e. in  $\Omega$  .

Now functions satisfying (2b) and (2c) are easily seen to form a closed convex set in  $\widetilde{H}^1(\Omega)$ . It is also easy to see that  $(J(u))^{\frac{1}{2}}$  is a norm in  $\widetilde{H}^1(\Omega)$ . This norm is in fact equivalent to the Sobolev norm in  $H^1(\Omega)$ :  $\|u\|^2 = J(u) + \int_{\Omega} u^2$  restricted to  $\widetilde{H}^1(\Omega)$ , as can be deduced from Poincare's inequality (see e.g. Dyn and Wahba [3]).

Thus (2) is the problem of finding the minimum norm element of a closed convex set in a Hilbert space, which always has a unique solution.

## 3. Variational characterization

For finite dimensional optimization, the solution is usually characterized by the famous Karush-Kuhn-Tucker conditions. There are extensions of the Kuhn-Tucker theorem to Banach space setting. We will use the following extension (Girsanov [4]): If Q is a closed convex set in a Banach space H, and  $J,h_1,\ldots,h_8$  are Frechet differentiable functions on H, then a necessary condition for u to minimize J(u) subject to  $u \in Q$ ,  $h_1(u) = a_1$ ,  $i = 1,\ldots,s$  is that there exist multipliers  $\lambda_1,\ldots,\lambda_n$ , such that

$$(\nabla J(u) + \sum_{i=1}^{8} \lambda_i \nabla h_i(u))(v-u) > 0, \quad \forall v \in Q .$$

Furthermore, if J is convex,  $h_1$ , i=1,...,s are linear and there exists  $u^*$  interior to Q satisfying  $h_1(u^*)=\alpha_1$ , i=1,...,s, then the above condition is also sufficient for  $u\in Q$  satisfying  $h_1(u)=\alpha_1$ , i=1,...,s to be the extremal solution.

To apply the above theorem to our problem, let  $J(u) = a(u,u) = \int_{\Omega} u_X^2 + u_Y^2$   $h_i(u) = \int_{\Omega} f_i u, \ Q = \{u \in H^*(\Omega), \ u > 0 \ \text{ a.e. in } \Omega\}, \ \text{ and } \ H = H^*(\Omega). \ \text{ The Frechet derivatives}$ are given by  $(\nabla J(u))(v) = a(u,v) \equiv \int_{\Omega} u_X^2 v_X + u_Y^2 v_Y \ \text{ and } \ (\nabla h_i(u))(v) = \int_{\Omega} f_i v, \ i = 1, \dots, s.$ 

By the above result, we obtain the following characterization of the solution to (1), for any set of constraints (1b) satisfied by at least one smooth positive function:

Theorem 2: u is the solution to (1) iff there exist multipliers  $\lambda_1, \dots, \lambda_g$  such that

$$a(u,v-u) > \int_{\Omega} f(v-u) \ \ \text{for all} \ \ v>0, \ \ v \in H^{1}(\Omega)$$
 (3a) 
$$\text{where} \ \ f = \sum_{i=1}^{S} \lambda_{i} f_{i} \ .$$

(3b) u > 0 a.e. in  $\Omega$ ,

(3c) 
$$\int_{\Omega} f_i u = \alpha_i, i = 1, \dots, s .$$

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By the same arguments we also obtain:

Lemma 1: Given  $\lambda_1, \dots, \lambda_s$  there is a unique function satisfying (3a) and (3b). This function minimizes  $J(u) = \int_{\Omega} (\sum_{i=1}^{s} \lambda_i f_i) u$  among all non-negative functions in  $H^1(\Omega)$ .

## 4. Local behaviour and boundary conditions

If in (1), we ignore the equality and inequality constraints, then the problem becomes a classical calculus of variation problem, the local behaviour of the solution will then be given by the Euler equation (vanishing of the first variation) and the natural boundary conditions. In our problem (1), which is constrained, we should expect to get a characterization of local behaviour similar to the Euler equation in the unconstrained case. We will show that, roughly speaking, when the constraints are not active in a certain neighbourhood, then the solution will satisfy a differential equation locally in the neighbourhood. This kind of local results are in general very difficult to prove, but our task is simplified considerably by some existing theorems on variational inequalities.

Lemma 2: Given  $f \in L^2(\Omega)$ , there exists a  $u \in H^2(\Omega)$ , satisfying the following variational inequality:

(4a) 
$$\int_{\Omega} (-\Delta \overline{u}) (v - \overline{u}) > \int_{\Omega} f(v - \overline{u}) \text{ for all } v > 0 \text{ a.e. in } \Omega, v \in H^{1}(\Omega) ,$$

(4b) 
$$\overline{u} > 0$$
 in  $\Omega$ ,

$$\frac{\partial \widetilde{u}}{\partial n} = 0 \quad \text{on} \quad \partial \Omega ,$$

where  $\Delta u = u_{xx} + u_{yy}$  is the Laplacian of u and  $\frac{\partial u}{\partial n}$  is the normal derivative at the boundary  $\partial \Omega$ .

<u>Proof:</u> This is a special case of theorem 1.12 in Brezis [2] (page 55), where we take  $\beta(r) \equiv 0$  ,  $-\infty < r < \infty$ , in applying that theorem.

This result is related to the solution of (1) in the following:

Lemma 3: Let  $\overline{u} \in H^2(\Omega)$  satisfy (4). Then  $\overline{u}$  satisfies also (3a).

Proof: Since  $\bar{u} \in H^2(\Omega)$ , we can use Green's formula<sup>1)</sup> to write

$$\int_{\Omega} \overline{u}_{x}(v-\overline{u})_{x} + \overline{u}_{y}(v-\overline{u})_{y} = \int_{\Omega} (-\Delta \overline{u})(v-\overline{u}) + \int_{\partial\Omega} \frac{\partial \overline{u}}{\partial n} (v-\overline{u}) .$$

The second integral in the right hand side vanishes, because the function  $\bar{u}$  satisfies the boundary conditions (4c). Therefore by (4a)

$$a(\overline{u},v-\overline{u}) = \int_{\Omega} (-\Delta \overline{u})(v-\overline{u}) > \int_{\Omega} f(v-\overline{u})$$
 for all  $v > 0$  a.e. in  $\Omega$ ,  $v \in H^{*}(\Omega)$ 

and u satisfies (3a).

Combining the results of Theorem 2 and Lemmas 1-3, we obtain a differential type necessary and sufficient condition for u to be the solution of (1).

Theorem 3: u is the solution to (1) iff the following conditions are satisfied:

(5a) 
$$u \in H^2(\Omega)$$

(5b) There exist  $\lambda_1, \dots, \lambda_g$  such that u satisfies

$$\int_{\Omega} (-\Delta u)(v-u) > \int_{\Omega} (\sum_{i=1}^{8} \lambda_{i} f_{i})(v-u) \quad \text{for all } v > 0 \quad \text{a.e. in } \Omega, v \in H^{\bullet}(\Omega) ,$$

See Aubin [1] for conditions required for Green's formula.

(5c) 
$$u > 0$$
 in  $\Omega$ 

(5d) 
$$\frac{\partial u}{\partial n} = 0$$
 on  $\partial \Omega$ 

(5e) 
$$\int_{\Omega} uf_{i} = \alpha_{i} , i = 1,...,s .$$

<u>Proof:</u> The sufficiency follows from Lemma 3 and Theorem 2. To prove the necessity of these conditions assume u to be the solution of (1). Then by Theorem 2, there exist  $\lambda_1, \dots, \lambda_8$  such that u satisfies (3a), and by Lemma 2, there exists  $\overline{u} \in H^2(\Omega)$  satisfying (5b), (5c), (5d), with  $\lambda_1, \dots, \lambda_8$  as in (3a). Hence by Lemma 3  $\overline{u}$  satisfies (3a) and (3b), which in view of Lemma 1 implies that  $\overline{u}$  coincides with u. This completes the proof of the theorem.

Property (5b) of the solution of (1) is equivalent to the following local behaviour in the distributional sense (Brezis [2]):

(5b) (-
$$\Delta u$$
) >  $\sum_{i=1}^{s} \lambda_i f_i$  in  $\Omega$ , (- $\Delta u$ ) =  $\sum_{i=1}^{s} \lambda_i f_i$  in  $\{x \in \Omega : u(x) > 0\}$ .

Moreover since  $u \in H^2(\Omega)$ ,  $\Delta u \in L^2(\Omega)$  and (5b)' holds almost everywhere in  $\Omega$ . Thus (5b)' in view of (5a) is equivalent to:

(5b)\* 
$$-\Delta u - \sum_{i=1}^{s} \lambda_i f_i > 0 \text{ a.e. in } \Omega, (-\Delta u - \sum_{i=1}^{s} \lambda_i f_i) u = 0 \text{ a.e. in } \Omega.$$

### 5. Problems of higher order

Similar analysis as done for problem (1) can be carried out for the more general problem related to the iterated Laplace operator:

(6a) 
$$\min_{\mathbf{u} \in \mathbf{H}^{\mathbf{m}}(\Omega)} J_{\mathbf{m}}(\mathbf{u}) = \int \int_{\Omega} \sum_{i=0}^{\mathbf{m}} {m \choose i} \left( \frac{\partial^{\mathbf{m}} \mathbf{u}}{\partial \mathbf{x}^{i} \partial^{\mathbf{m}-i} \mathbf{y}} \right)^{2}$$

subject to

(6b) 
$$\int u f_{\underline{i}} = \alpha_{\underline{i}} , \quad \underline{i} = 1, ..., s$$

(6c) 
$$u > 0$$
 in  $\Omega$ ,

where  $\Omega$  is a smooth region in  $\mathbb{R}^2$ ,  $\mathbf{f_i} \in L^2(\Omega)$ , i = 1, ..., s, and  $\mathbf{H}^m(\Omega)$  is the m'th order Sobolev space

$$H^{m}(\Omega) = \{u \mid \frac{\partial^{k} u}{\partial x^{i} \partial y^{k-i}} \in L^{2}(\Omega), i = 0,...,k, k = 0,...,m\}$$

For m > 2 all functions in  $\operatorname{H}^m(\Omega)$  are continuous, and the positivity in (6c) is pointwise.

For this problem we obtain analogous results to Theorem 1,2 for the case m=1, for sets of linear constraints (6b) satisfying the following two assumptions:

- (i) There exists a smooth positive function satisfying (6b).
- (ii) There does not exist a polynomial q of total degree k, k < m, satisfying  $\int_{C} f_{i}q = 0, i = 1,...,s.$

The existence, uniqueness and characterization in terms of a variational inequality are derived by the same arguments used in Sections 2,3. We formulate the results and omit the proofs.

Theorem 4: There exists a unique solution to problem (6). u is the solution to (6) iff there exist multipliers  $\lambda_1, \ldots, \lambda_q$  such that

(7a) 
$$a_{m}(u, v-u) > \int_{\Omega} (v-u) \sum_{i=1}^{s} \lambda_{i} f_{i} \text{ for all } v > 0, v \in H^{m}(\Omega)$$

(7b) 
$$u > 0$$
 in  $\Omega$ 

(7c) 
$$\int_{\Omega} f_{\underline{i}} u = \alpha_{\underline{i}} , \quad \underline{i} = 1, \dots, s .$$

where

(8) 
$$a_{m}(u,v) = \int_{\Omega} \sum_{i=0}^{m} {m \choose i} \frac{\partial^{m} u}{\partial x^{i} \partial y^{m-i}} \frac{\partial^{m} v}{\partial x^{i} \partial y^{m-i}}.$$

In order to conclude local and boundary behaviour of the solution to (6), an extension of Brezis' result (Lemma 2) to m > 2 is needed. At this stage the extension of Theorem 3 to m > 2 is yet a conjecture:

Conjecture: u is the solution to (6) iff the following conditions are satisfied

(9a) 
$$u \in H^{2m}(\Omega)$$

(9b) There exist  $\lambda_1, \dots, \lambda_g$  such that u satisfies

$$(-1)^{\mathfrak{m}} \, \int_{\Omega} \, \Delta^{\mathfrak{m}} u(v-u) \, \geq \, \int_{\Omega} \, \Big( \sum_{\mathbf{i}=1}^{\mathbf{s}} \, \lambda_{\mathbf{i}} \, \mathbf{f}_{\mathbf{i}} \, \Big) (v-u) \quad \text{for all} \quad v \, > \, 0 \, , \, \, v \, \in \, \mathbf{H}^{\mathfrak{m}}(\Omega) \quad ,$$

(9c) 
$$u > 0$$
 in  $\Omega$ 

(9d) 
$$\delta_{2m-i} u = 0 \text{ on } \partial\Omega$$
,  $i = 1, ..., m$ 

(9e) 
$$\int_{\Omega} uf_{i} = \alpha_{i} , \quad i = 1,...,s$$

where  $\delta_{2m-i}$ , i = 1,...,m are differential operators of order 2m-i defined by the generalized Green's formula (Aubin [1]):

(10) 
$$a_{m}(u,v) = (-1)^{m} \int_{\Omega} (\Delta^{m}u)v + \sum_{i=0}^{m-1} \int_{\partial\Omega} (\delta_{2m-1-i}u) \frac{3^{i}}{\partial n^{i}} v .$$

The local behaviour of u in  $\Omega$  implied by (9a) and (9b) is:

(11a) 
$$(-1)^m \Delta^m u > \sum_{i=1}^n \lambda_i f_i \quad \text{a.e. in } \Omega$$

(11b) 
$$[(-1)^m \Delta^m \mathbf{u} - \sum_{i=1}^s \lambda_i f_i] \cdot \mathbf{u} = 0 \text{ a.e. in } \Omega .$$

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